Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

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Chemical Analysis of Simulated High Level Waste Glasses to Support Stage III Sulfate Solubility Modeling

K. M. Fox

March 2016

SRNL-STI-2016-00109, Revision 0

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Prepared for
U.S. Department of Energy

SRNL-STI-2016-00109
Revision 0

Keywords: *High level waste glass, sulfur solubility, modeling*

Retention: *Permanent*

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ACKNOWLEDGEMENTS

The author thanks Phyllis Workman, Madison Caldwell, Kim Wyszynski, Beverly Wall, and Whitney Riley at Savannah River National Laboratory for their assistance with the laboratory analyses described in this report. Funding from the U.S. Department of Energy – Office of Environmental Management via the International Cooperation Program is gratefully acknowledged.

EXECUTIVE SUMMARY

The U.S. Department of Energy (DOE), Office of Environmental Management is sponsoring an international, collaborative project to develop a fundamental model for sulfate solubility in nuclear waste glass. The solubility of sulfate has a significant impact on the achievable waste loading for nuclear waste forms within the DOE complex.

A fundamental model of sulfate solubility in glass, under development at Sheffield Hallam University (SHU), could provide a solution to the issues of sulfate solubility in glass. The model uses the normalized cation field strength index as a function of glass composition to predict sulfate capacity, and has shown early success for some glass systems. The objective of the current scope at SHU is to mature the sulfate solubility model to the point where it can be used to guide glass composition development, allowing for enhanced waste loadings and waste throughput. A series of targeted glass compositions was selected to resolve data gaps in the model and is identified as Stage III. SHU fabricated these glasses and sent samples to SRNL for chemical composition analysis. SHU will use the resulting data to enhance the sulfate solubility model and resolve any deficiencies.

Chemical composition analysis was performed on a representative sample of each of the Stage III study glasses. Three preparation techniques, sodium peroxide fusion, lithium metaborate fusion, and potassium hydroxide fusion, were used to prepare the glass samples for analysis. Each of the prepared samples was analyzed twice to obtain measurements for each element of interest. An average value was computed for each component on an oxide basis. The resulting measurements were compared with the targeted values. Some differences between the targeted and measured compositions were identified. It is therefore recommended that the measured compositions, rather than targeted compositions, be used to support the sulfate solubility modeling effort for these glasses.

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LIST OF ABBREVIATIONS

DOE	U.S. Department of Energy
DWPF	Defense Waste Processing Facility
EM	Environmental Management
HLW	High Level Waste
IC	Ion Chromatography
ICP-OES	Inductively Coupled Plasma – Optical Emission Spectroscopy
KH	Potassium Hydroxide Fusion
LAW	Low Activity Waste
LM	Lithium Metaborate Fusion
PF	Sodium Peroxide Fusion
PNNL	Pacific Northwest National Laboratory
SHU	Sheffield Hallam University
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
wt %	Weight Percent
WTP	Hanford Tank Waste Treatment and Immobilization Plant

1.0 Introduction

The U.S. Department of Energy (DOE), Office of Environmental Management (EM) is sponsoring an international, collaborative project to develop a fundamental model for sulfate solubility in nuclear waste glass. The solubility of sulfate has a significant impact on the achievable waste loading for nuclear waste forms within the DOE complex. These wastes can contain relatively high concentrations of sulfate, which has low solubility in borosilicate glass.[1] This is a significant issue for low activity waste (LAW) glass and is projected to have a major impact on the Hanford Tank Waste Treatment and Immobilization Plant (WTP). Sulfate solubility has also been a limiting factor for recent high level waste (HLW) sludge processed at the Savannah River Site (SRS) Defense Waste Processing Facility (DWPF).[2-5] The low solubility of sulfate in glass, along with melter and off-gas corrosion constraints, dictate that the waste be blended with lower sulfate concentration waste sources or washed to remove sulfate prior to vitrification. The development of enhanced borosilicate glass compositions with improved sulfate solubility will allow for higher waste loadings and accelerate mission completion.

Studies at Savannah River National Laboratory (SRNL) in support of the DWPF have identified frit additives that can be used to marginally improve sulfate solubility in simulated waste glasses.[6] However, due to the complexity of SRS waste compositions, much of this work has been done on an empirical basis,[2,5] making it difficult to apply the findings to future waste compositions despite the large number of glass systems studied.[7] Researchers at the Pacific Northwest National Laboratory (PNNL) have completed extensive glass formulation studies to evaluate the solubility of sulfate in glass compositions for Hanford wastes, although the empirical nature of these studies makes it difficult to apply the results to anticipated compositions to be processed in the WTP. A more fundamental, rather than empirical, model of sulfate solubility in glass, under development at Sheffield Hallam University (SHU), could provide a solution to the issues of sulfate solubility. The model uses the normalized cation field strength index as a function of glass composition to predict sulfate capacity, and has shown early success for some glass systems.[8]

Through previous DOE-EM International Program funding, the combination of this model with the data collected at SRNL resulted in positive model correlations for sulfate solubility in borosilicate waste glasses.[9] Utilizing funding obtained in late FY12, an extensive data set covering LAW and HLW glasses developed at PNNL and the Vitreous State Laboratory at Catholic University was compiled and transmitted to SHU for incorporation into the model. These data will significantly expand the coverage of the model given the compositional differences between HLW and LAW glasses.

The objective of the current scope being pursued by SHU is to mature the sulfate solubility model to the point where it can be used to guide glass composition development for DWPF and WTP, allowing for enhanced waste loadings and waste throughput at these facilities. A series of targeted glass compositions was selected to resolve data gaps in the model and is identified as Stage III.[10] SHU fabricated these glasses and sent samples to SRNL for chemical composition analysis. SHU will use the resulting data to enhance the sulfate solubility model and resolve any deficiencies. In this report, SRNL provides chemical analyses for the Stage III, simulated HLW glasses fabricated by SHU in support of the sulfate solubility model development.

2.0 Experimental Procedure

2.1 Chemical Composition Analysis

Chemical analysis was performed on a representative sample from each of the study glasses to allow for comparisons with the targeted compositions. Two preparation techniques, sodium peroxide fusion (PF) and lithium metaborate fusion (LM) were used to prepare the glass samples for analysis. Each of the

prepared samples was analyzed, twice for each element of interest, by inductively coupled plasma – optical emission spectroscopy (ICP-OES). Additional samples of those glasses that contained chlorine were prepared by potassium hydroxide fusion (KH) and analyzed by ion chromatography (IC) to determine the concentration of chloride ion in the glass.

2.2 Quality Assurance

Requirements for performing reviews of technical reports and the extent of review are established in manual Savannah River Site Manual E7 2.60. SRNL documents the extent and type of review using the SRNL Technical Report Design Checklist contained in WSRC-IM-2002-00011, Rev. 2. Laboratory data for this study were recorded in the SRNL Electronic Laboratory Notebook system, experiment C3489-00224-01.

3.0 Results and Discussion

The measurements for each sample as prepared and measured in duplicate are given in Table A-1 in Appendix A, and are as reported by the analytical laboratory in units of elemental weight percent (wt %). The average of each pair of measured values was computed and multiplied by the appropriate gravimetric factor to arrive at the measured compositions for each of the study glasses, as oxides (or chlorine). During the process of converting to oxide concentrations, an elemental concentration that was reported to be below the detection limit of the analytical process (for an element that was included in the targeted composition) was set to the detection limit as the oxide concentration was determined for the purpose of calculating a sum of oxides for each glass. Those oxides with measured concentrations that were below the associated detection limit are denoted with a less than symbol (<) as the measured compositions are reported.

The average measured compositions of the Stage III study glasses are reported in Table 4-1 through Table 4-4. All of the measured sums of oxides for the study glasses fall within the interval of 98.6 to 102.9 wt %, indicating good recovery of all components. Table A-2 in Appendix A provides a summary of the average compositions as well as the targeted compositions and their relative percent differences.

Some observations of the measured versus targeted compositions are offered. For the HLW series glasses:

- Glasses HLW5, HLW6, HLW8, and HLW10, have measured Al_2O_3 concentrations that are below the targeted values.
- The glasses are generally low in B_2O_3 relative to the targeted concentrations.
- Glass HLW0 is high in Cr_2O_3 relative to the targeted value.
- The measured MgO concentrations in glasses HLW10 and HLW11 are above the targeted values.
- The measured sulfate concentrations are generally lower than the targeted values, as expected since there was an unincorporated sulfate phase visible on the glasses after fabrication.
- The measured SiO_2 values are generally greater than the targeted values.
- The measured ZnO concentrations for glasses HLW8 and HLW9 are below the targeted values.

For the S+Cl series glasses:

- The measured concentrations of Al_2O_3 are generally greater than the targeted values.
- The measured B_2O_3 concentrations are relatively close to the targeted values, as compared to the other sets of glasses in this study.
- The measured Cl concentrations are low relative to the targeted values, with the differences increasing as the targeted Cl concentration increases.
- The measured sulfate concentrations are generally lower than the targeted values, as expected since there was an unincorporated sulfate phase visible on the glasses after fabrication.
- The measured SiO_2 concentrations are generally greater than the targeted values.

- The measured ZrO_2 concentrations are below the targeted values.

For the S+V series glasses:

- The measured Al_2O_3 concentrations are generally above the targeted values.
- The glasses are generally low in B_2O_3 and ZrO_2 relative to the targeted concentrations.
- The measured sulfate concentrations are generally lower than the targeted values, as expected. Glass SV 4 is an exception, with a measured sulfate concentration that is higher than the targeted value.
- The measured SiO_2 concentrations are generally greater than the targeted values.
- The measured ZrO_2 concentrations are below the targeted values.

For the S+Fe series glasses:

- The measured Al_2O_3 concentrations are generally above the targeted values.
- The glasses are generally low in B_2O_3 relative to the targeted concentrations.
- The measured sulfate concentrations are generally lower than the targeted values, as expected since there was an unincorporated sulfate phase visible on the glasses after fabrication.
- The measured SiO_2 concentrations are generally greater than the targeted values.
- The measured ZrO_2 concentrations are below the targeted values.

4.0 Summary

Chemical composition analysis was performed on a representative sample of each of the Stage III study glasses. Three preparation techniques, sodium peroxide fusion, lithium metaborate fusion, and potassium hydroxide fusion, were used to prepare the glass samples for analysis. Each of the prepared samples was analyzed twice by ICP-OES or IC to obtain measurements for each element of interest. An average value was computed for each component on an oxide basis. The resulting measurements were compared with the targeted values. Some differences between the targeted and measured compositions were identified. It is therefore recommended that the measured compositions, rather than targeted compositions, be used to support the sulfate solubility modeling effort for these glasses.

Table 4-1. Measured Compositions (wt %) of the HLW Series Glasses

Glass ID	Al_2O_3	B_2O_3	BaO	CaO	Cr_2O_3	Fe_2O_3	Li_2O	MgO	MnO	Na_2O	P_2O_5	SO_3	SiO_2	ZnO	Sum
HLW0	9.56	4.69	<0.112	5.08	0.501	9.98	4.99	0.185	1.90	15.2	0.947	0.306	47.4	<0.124	101.0
HLW1	9.92	4.38	<0.112	5.27	0.285	9.61	4.85	<0.166	1.78	14.3	0.931	1.30	48.1	<0.124	101.1
HLW2	9.83	4.24	<0.112	4.94	0.355	10.1	8.43	<0.166	1.76	7.39	0.984	1.66	50.6	<0.124	100.7
HLW3	10.1	4.75	<0.112	5.44	0.272	10.8	13.4	<0.166	1.92	0.231	1.08	2.30	52.2	<0.124	102.9
HLW4	9.84	4.15	<0.112	4.97	0.276	9.76	2.31	<0.166	1.75	19.2	0.880	1.10	47.1	<0.124	101.7
HLW5	7.67	4.49	<0.112	4.82	0.249	9.55	2.28	<0.166	1.74	22.5	0.835	1.05	44.8	<0.124	100.4
HLW6	8.32	4.00	7.08	2.47	0.290	9.62	4.67	<0.166	1.72	13.7	0.920	1.23	46.5	<0.124	100.8
HLW7	8.67	3.52	13.3	<0.14	0.259	9.04	4.36	<0.166	1.64	13.6	0.825	0.627	44.6	<0.124	100.9
HLW8	7.93	4.13	<0.112	2.54	0.311	10.0	4.82	<0.166	1.76	14.4	0.913	1.10	49.2	3.01	100.4
HLW9	9.22	3.95	<0.112	<0.14	0.313	9.51	4.65	<0.166	1.71	14.0	0.885	0.869	48.0	5.26	98.8
HLW10	7.46	4.43	<0.112	2.6	0.303	10.0	4.89	3.01	1.95	14.6	0.944	1.09	48.8	<0.124	100.3
HLW11	9.92	3.99	<0.112	0.181	0.286	9.45	4.70	5.29	1.68	14.0	0.968	0.859	47.0	<0.124	98.6

Table 4-2. Measured Compositions (wt %) of the S+Cl Series Glasses

Glass ID	Al_2O_3	B_2O_3	CaO	Fe_2O_3	Li_2O	Na_2O	SO_3	SiO_2	ZrO_2	Cl	Sum
SCl 1	6.14	5.87	6.70	14.8	4.98	12.4	1.14	48.5	0.879	0.135	101.5
SCl 2	6.18	6.06	6.64	14.4	4.95	12.4	1.13	48.1	0.807	0.229	100.9
SCl 3	6.24	5.94	6.39	14.6	4.89	12.5	1.08	47.9	0.838	0.318	100.7
SCl 4	6.24	6.07	6.58	14.6	4.88	12.6	1.04	47.8	0.845	0.421	101.1
SCl 5	7.20	5.97	6.39	14.1	4.83	12.6	0.835	47.6	0.807	0.777	101.1
A3=B3+S	6.34	6.18	6.46	14.3	4.97	12.0	1.12	48.1	0.889	-	100.4

Table 4-3. Measured Compositions (wt %) of the S+V Series Glasses

Glass ID	Al_2O_3	B_2O_3	CaO	Fe_2O_3	Li_2O	Na_2O	SO_3	SiO_2	V_2O_5	ZrO_2	Sum
SV 1	6.47	4.87	6.67	15.0	4.54	12.1	1.50	46.6	2.35	0.833	100.9
SV 2	5.84	4.76	5.76	13.8	4.47	11.7	1.68	48.0	4.42	0.841	101.3
SV 3	5.94	4.37	5.89	12.8	4.19	11.4	1.79	48.0	6.34	0.731	101.5
SV 4	5.90	4.29	6.25	14.0	4.46	11.2	2.23	44.3	9.33	0.819	102.8
A3B3+S	6.53	4.90	6.79	15.2	4.70	12.2	1.23	47.7	-	0.921	100.2

Table 4-4. Measured Compositions (wt %) of the S+Fe Series Glasses

Glass ID	Al_2O_3	B_2O_3	CaO	Fe_2O_3	Li_2O	Na_2O	SO_3	SiO_2	ZrO_2	Sum
S Fe 1	6.92	4.97	6.80	13.6	4.83	12.4	1.28	49.1	0.929	100.8
S Fe 2	7.17	5.12	6.99	10.9	5.00	13.0	1.29	50.8	0.960	101.2
S Fe 3	7.43	5.36	7.33	8.15	5.19	13.6	1.30	52.3	1.01	101.7
S Fe 4	6.91	5.39	7.51	5.33	5.36	13.8	1.54	53.8	0.995	100.6

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Appendix A Tables and Exhibits Supporting the Chemical Composition Measurements

Table A-1. Measurements of the Stage III Sulfate Study Glasses in wt %

Sample ID	Meas.	Al	B	Ba	Ca	Cl	Cr	Fe	Li	Mg	Mn	Na	P	S	Si	V	Zn	Zr
HLW0	1	5.06	1.49	<0.100	3.63	-	0.342	6.99	2.32	0.111	1.47	11.3	0.414	0.123	22.2	<0.100	<0.100	<0.100
HLW0	2	5.06	1.42	<0.100	3.63	-	0.344	6.97	2.31	0.112	1.47	11.2	0.412	0.123	22.1	<0.100	<0.100	<0.100
HLW1	1	5.27	1.38	<0.100	3.78	-	0.196	6.74	2.25	<0.100	1.38	10.7	0.406	0.516	22.5	<0.100	<0.100	<0.100
HLW1	2	5.23	1.34	<0.100	3.75	-	0.195	6.69	2.25	<0.100	1.37	10.6	0.407	0.523	22.5	<0.100	<0.100	<0.100
HLW2	1	5.19	1.34	<0.100	3.53	-	0.242	7.08	3.91	<0.100	1.36	5.47	0.428	0.666	23.6	<0.100	<0.100	<0.100
HLW2	2	5.21	1.30	<0.100	3.53	-	0.243	7.08	3.92	<0.100	1.36	5.51	0.431	0.668	23.7	<0.100	<0.100	<0.100
HLW3	1	5.31	1.49	<0.100	3.87	-	0.186	7.53	6.20	<0.100	1.49	0.171	0.471	0.917	24.2	<0.100	<0.100	<0.100
HLW3	2	5.34	1.47	<0.100	3.90	-	0.186	7.58	6.25	<0.100	1.49	0.172	0.474	0.927	24.5	<0.100	<0.100	<0.100
HLW4	1	5.21	1.31	<0.100	3.55	-	0.189	6.83	1.07	<0.100	1.36	14.2	0.385	0.438	22.1	<0.100	<0.100	<0.100
HLW4	2	5.21	1.26	<0.100	3.55	-	0.188	6.82	1.07	<0.100	1.35	14.2	0.383	0.441	21.9	<0.100	<0.100	<0.100
HLW5	1	4.04	1.41	<0.100	3.43	-	0.170	6.63	1.06	<0.100	1.34	16.6	0.366	0.421	20.9	<0.100	<0.100	<0.100
HLW5	2	4.07	1.38	<0.100	3.45	-	0.171	6.73	1.06	<0.100	1.36	16.8	0.363	0.423	21.0	<0.100	<0.100	<0.100
HLW6	1	4.41	1.28	6.38	1.77	-	0.199	6.74	2.18	<0.100	1.33	10.2	0.401	0.493	21.9	<0.100	<0.100	<0.100
HLW6	2	4.40	1.20	6.30	1.76	-	0.199	6.72	2.16	<0.100	1.33	10.2	0.402	0.491	21.6	<0.100	<0.100	<0.100
HLW7	1	4.59	1.11	11.9	<0.100	-	0.177	6.33	2.03	<0.100	1.27	10.1	0.359	0.250	20.9	<0.100	<0.100	<0.100
HLW7	2	4.59	1.08	11.9	<0.100	-	0.177	6.31	2.01	<0.100	1.27	10.1	0.361	0.252	20.7	<0.100	<0.100	<0.100
HLW8	1	4.18	1.31	<0.100	1.81	-	0.212	6.95	2.26	<0.100	1.35	10.6	0.397	0.437	23.2	<0.100	2.38	<0.100
HLW8	2	4.22	1.26	<0.100	1.83	-	0.214	7.06	2.22	<0.100	1.37	10.8	0.401	0.444	22.8	<0.100	2.45	<0.100
HLW9	1	4.91	1.23	<0.100	<0.100	-	0.214	6.68	2.16	<0.100	1.33	10.4	0.387	0.346	22.4	<0.100	4.21	<0.100
HLW9	2	4.85	1.23	<0.100	<0.100	-	0.214	6.62	2.17	<0.100	1.32	10.3	0.385	0.350	22.5	<0.100	4.25	<0.100
HLW10	1	3.94	1.44	<0.100	1.86	-	0.207	6.99	2.26	1.81	1.51	10.8	0.410	0.438	22.7	<0.100	<0.100	<0.100
HLW10	2	3.96	1.32	<0.100	1.87	-	0.207	7.00	2.28	1.82	1.51	10.8	0.414	0.438	23.0	<0.100	<0.100	<0.100
HLW11	1	5.28	1.26	<0.100	0.130	-	0.196	6.65	2.19	3.19	1.31	10.4	0.421	0.338	22.0	<0.100	<0.100	<0.100
HLW11	2	5.22	1.22	<0.100	0.129	-	0.196	6.57	2.18	3.19	1.29	10.3	0.424	0.350	21.9	<0.100	<0.100	<0.100
SV 1	1	3.43	1.48	<0.100	4.78	-	<0.010	10.5	2.09	<0.100	<0.100	9.00	<0.100	0.592	21.5	1.31	<0.100	0.615
SV 1	2	3.41	1.55	<0.100	4.75	-	<0.010	10.5	2.13	<0.100	<0.100	8.95	<0.100	0.606	22.1	1.32	<0.100	0.618
SV 2	1	3.10	1.48	<0.100	4.14	-	0.012	9.66	2.07	<0.100	<0.100	8.73	<0.100	0.674	22.4	2.48	<0.100	0.624
SV 2	2	3.07	1.48	<0.100	4.09	-	0.012	9.59	2.08	<0.100	<0.100	8.59	<0.100	0.669	22.5	2.47	<0.100	0.622
SV 3	1	3.14	1.36	<0.100	4.21	-	0.021	9.00	1.94	<0.100	<0.100	8.49	<0.100	0.710	22.3	3.55	<0.100	0.538
SV 3	2	3.14	1.35	<0.100	4.20	-	0.022	8.96	1.95	<0.100	<0.100	8.42	<0.100	0.724	22.5	3.56	<0.100	0.545
SV 4	1	3.14	1.33	<0.100	4.49	-	0.014	9.87	2.07	<0.100	<0.100	8.38	<0.100	0.895	20.6	5.24	<0.100	0.608
SV 4	2	3.11	1.34	<0.100	4.45	-	0.014	9.78	2.08	<0.100	<0.100	8.31	<0.100	0.892	20.8	5.21	<0.100	0.605
A3B3+S	1	3.47	1.54	<0.100	4.87	-	0.012	10.6	2.18	<0.100	<0.100	9.06	<0.100	0.493	22.3	<0.100	<0.100	0.680
A3B3+S	2	3.45	1.51	<0.100	4.83	-	0.012	10.6	2.18	<0.100	<0.100	9.06	<0.100	0.494	22.2	<0.100	<0.100	0.684
S Fe 1	1	3.65	1.55	<0.100	4.84	-	0.083	9.52	2.25	<0.100	<0.100	9.19	<0.100	0.513	23.0	<0.100	<0.100	0.685
S Fe 1	2	3.68	1.54	<0.100	4.88	-	0.083	9.56	2.24	<0.100	<0.100	9.28	<0.100	0.516	22.9	<0.100	<0.100	0.691

Table A-1. Measurements of the Stage III Sulfate Study Glasses in wt % (continued)

Sample ID	Meas.	Al	B	Ba	Ca	Cl	Cr	Fe	Li	Mg	Mn	Na	P	S	Si	V	Zn	Zr
S Fe 2	1	3.78	1.57	<0.100	4.98	-	0.077	7.58	2.32	<0.100	<0.100	9.63	<0.100	0.516	23.7	<0.100	<0.100	0.708
S Fe 2	2	3.80	1.61	<0.100	5.01	-	0.078	7.63	2.32	<0.100	<0.100	9.67	<0.100	0.518	23.8	<0.100	<0.100	0.714
S Fe 3	1	3.95	1.67	<0.100	5.27	-	0.082	5.73	2.41	<0.100	<0.100	10.1	<0.100	0.524	24.5	<0.100	<0.100	0.750
S Fe 3	2	3.92	1.66	<0.100	5.20	-	0.081	5.67	2.41	<0.100	<0.100	10.0	<0.100	0.521	24.4	<0.100	<0.100	0.742
S Fe 4	1	3.67	1.69	<0.100	5.40	-	0.080	3.74	2.50	<0.100	<0.100	10.3	<0.100	0.610	25.3	<0.100	<0.100	0.735
S Fe 4	2	3.64	1.65	<0.100	5.34	-	0.080	3.71	2.48	<0.100	<0.100	10.2	<0.100	0.627	25.0	<0.100	<0.100	0.738
SCl 1	1	3.24	1.83	-	4.77	0.135	-	10.4	2.31	-	-	9.15	-	0.454	22.6	-	-	0.640
SCl 1	2	3.26	1.81	-	4.81	0.135	-	10.4	2.31	-	-	9.20	-	0.457	22.7	-	-	0.661
SCl 2	1	3.27	1.88	-	4.75	0.229	-	10.1	2.30	-	-	9.20	-	0.454	22.4	-	-	0.597
SCl 2	2	3.27	1.88	-	4.75	0.229	-	10.1	2.30	-	-	9.17	-	0.452	22.5	-	-	0.598
SCl 3	1	3.29	1.84	-	4.55	0.319	-	10.2	2.28	-	-	9.21	-	0.433	22.5	-	-	0.622
SCl 3	2	3.31	1.84	-	4.58	0.317	-	10.3	2.26	-	-	9.27	-	0.429	22.3	-	-	0.618
SCl 4	1	3.30	1.85	-	4.69	0.422	-	10.2	2.25	-	-	9.35	-	0.414	22.1	-	-	0.618
SCl 4	2	3.31	1.91	-	4.72	0.420	-	10.3	2.29	-	-	9.41	-	0.417	22.6	-	-	0.632
SCl 5	1	3.82	1.88	-	4.57	0.778	-	9.85	2.25	-	-	9.35	-	0.333	22.3	-	-	0.581
SCl 5	2	3.80	1.83	-	4.56	0.776	-	9.81	2.24	-	-	9.32	-	0.335	22.2	-	-	0.613
A3=B3+S	1	3.35	1.92	-	4.62	-	-	9.99	2.31	-	-	8.88	-	0.451	22.5	-	-	0.658
A3=B3+S	2	3.36	1.92	-	4.62	-	-	9.99	2.30	-	-	8.93	-	0.446	22.4	-	-	0.658

Table A-2. Comparison of Targeted and Measured Compositions (wt %) of the Study Glasses

ID	Type	Al_2O_3	B_2O_3	BaO	CaO	Cl	Cr_2O_3	Fe_2O_3	Li_2O	MgO	MnO	Na_2O	P_2O_5	SO_3	SiO_2	V_2O_5	ZnO	ZrO_2
HLW0	Target	10.204	5.102	0	5.102	-	0.255	10.204	5.102	0	1.786	15.306	1.02	-	45.918	-	0	-
	Meas.	9.56	4.69	<0.112	5.08	-	0.501	9.98	4.99	0.185	1.90	15.2	0.947	0.306	47.4	-	<0.124	-
	% Err	-6.3	-8.1	-	-0.4	-	96.5	-2.2	-2.2	-	6.4	-0.7	-7.2	-	3.2	-	-	-
HLW1	Target	10	5	0	5	-	0.25	10	5	0	1.75	15	1	2	45	-	0	-
	Meas.	9.92	4.38	<0.112	5.27	-	0.285	9.61	4.85	<0.166	1.78	14.3	0.931	1.30	48.1	-	<0.124	-
	% Err	-0.8	-12.4	-	5.4	-	14.0	-3.9	-3.0	-	1.7	-4.7	-6.9	-35.0	6.9	-	-	-
HLW2	Target	10.404	5.202	0	5.202	-	0.26	10.404	8.965	0	1.821	7.803	1.04	2.081	46.818	-	0	-
	Meas.	9.83	4.24	<0.112	4.94	-	0.355	10.1	8.43	<0.166	1.76	7.39	0.984	1.66	50.6	-	<0.124	-
	% Err	-5.5	-18.5	-	-5.0	-	36.5	-2.9	-6.0	-	-3.3	-5.3	-5.4	-20.2	8.1	-	-	-
HLW3	Target	10.842	5.421	0	5.421	-	0.271	10.842	13.263	0	1.897	0	1.084	2.168	48.791	-	0	-
	Meas.	10.1	4.75	<0.112	5.44	-	0.272	10.8	13.4	<0.166	1.92	0.231	1.08	2.30	52.2	-	<0.124	-
	% Err	-6.8	-12.4	-	0.4	-	0.4	-0.4	1.0	-	1.2	-	-0.4	6.1	7.0	-	-	-
HLW4	Target	9.739	4.869	0	4.869	-	0.244	9.738	2.435	0	1.704	19.658	0.974	1.948	43.822	-	0	-
	Meas.	9.84	4.15	<0.112	4.97	-	0.276	9.76	2.31	<0.166	1.75	19.2	0.880	1.10	47.1	-	<0.124	-
	% Err	1.0	-14.8	-	2.1	-	13.1	0.2	-5.1	-	2.7	-2.3	-9.7	-43.5	7.5	-	-	-
HLW5	Target	9.49	4.745	0	4.745	-	0.237	9.49	0	0	1.661	24.079	0.949	1.898	42.706	-	0	-
	Meas.	7.67	4.49	<0.112	4.82	-	0.249	9.55	2.28	<0.166	1.74	22.5	0.835	1.05	44.8	-	<0.124	-
	% Err	-19.2	-5.4	-	1.6	-	5.1	0.6	-	-	4.8	-6.6	-12.0	-44.7	4.9	-	-	-
HLW6	Target	9.585	4.792	6.551	2.396	-	0.24	9.584	4.793	0	1.677	14.377	0.958	1.917	43.13	-	0	-
	Meas.	8.32	4.00	7.08	2.47	-	0.290	9.62	4.67	<0.166	1.72	13.7	0.920	1.23	46.5	-	<0.124	-
	% Err	-13.2	-16.5	8.1	3.1	-	20.8	0.4	-2.6	-	2.6	-4.7	-4.0	-35.8	7.8	-	-	-
HLW7	Target	9.202	4.601	12.58	0	-	0.23	9.202	4.602	0	1.61	13.803	0.92	1.84	41.41	-	0	-
	Meas.	8.67	3.52	13.3	<0.140	-	0.259	9.04	4.36	<0.166	1.64	13.6	0.825	0.627	44.6	-	<0.124	-
	% Err	-5.8	-23.5	5.7	-	-	12.6	-1.8	-5.3	-	1.9	-1.5	-10.3	-65.9	7.7	-	-	-
HLW8	Target	9.888	4.944	0	2.472	-	0.247	9.888	4.945	0	1.731	14.832	0.989	1.978	44.497	-	3.589	-
	Meas.	7.93	4.13	<0.112	2.54	-	0.311	10.0	4.82	<0.166	1.76	14.4	0.913	1.10	49.2	-	3.01	-
	% Err	-19.8	-16.5	-	2.8	-	25.9	1.1	-2.5	-	1.7	-2.9	-7.7	-44.4	10.6	-	-16.1	-
HLW9	Target	9.779	4.89	0	0	-	0.245	9.779	4.89	0	1.711	14.669	0.978	1.956	44.005	-	7.098	-
	Meas.	9.22	3.95	<0.112	<0.140	-	0.313	9.51	4.65	<0.166	1.71	14.0	0.885	0.869	48.0	-	5.26	-
	% Err	-5.7	-19.2	-	-	-	27.8	-2.8	-4.9	-	-0.1	-4.6	-9.5	-55.6	9.1	-	-25.9	-
HLW10	Target	10.071	5.035	0	2.518	-	0.252	10.071	5.036	1.81	1.762	15.106	1.007	2.014	45.318	-	0	-
	Meas.	7.46	4.43	<0.112	2.60	-	0.303	10.0	4.89	3.01	1.95	14.6	0.944	1.09	48.8	-	<0.124	-
	% Err	-25.9	-12.0	-	3.3	-	20.2	-0.7	-2.9	66.3	10.7	-3.3	-6.3	-45.9	7.7	-	-	-
HLW11	Target	10.143	5.071	0	0	-	0.254	10.142	5.072	3.645	1.775	15.214	1.014	2.029	45.641	-	0	-
	Meas.	9.92	3.99	<0.112	0.181	-	0.286	9.45	4.70	5.29	1.68	14.0	0.968	0.859	47.0	-	<0.124	-
	% Err	-2.2	-21.3	-	-	-	12.6	-6.8	-7.3	45.1	-5.4	-8.0	-4.5	-57.7	3.0	-	-	-

Table A-2. Comparison of Targeted and Measured Compositions (wt %) of the Study Glasses (continued)

ID	Type	Al_2O_3	B_2O_3	BaO	CaO	Cl	Cr_2O_3	Fe_2O_3	Li_2O	MgO	MnO	Na_2O	P_2O_5	SO_3	SiO_2	V_2O_5	ZnO	ZrO_2
SCl 1	Target	5.922	5.922	-	6.910	0.152	-	15.793	4.935	-	-	12.964	-	1.999	44.417	-	-	0.987
	Meas.	6.14	5.87	-	6.7	0.135	-	14.8	4.98	-	-	12.4	-	1.14	48.5	-	-	0.879
	% Err	3.7	-0.9	-	-3.0	-11.0	-	-6.3	0.9	-	-	-4.4	-	-43.0	9.2	-	-	-10.9
SCl 2	Target	5.905	5.905	-	6.889	0.303	-	15.747	4.921	-	-	13.059	-	1.999	44.288	-	-	0.984
	Meas.	6.18	6.06	-	6.64	0.229	-	14.4	4.95	-	-	12.4	-	1.13	48.1	-	-	0.807
	% Err	4.7	2.6	-	-3.6	-24.4	-	-8.6	0.6	-	-	-5.0	-	-43.5	8.6	-	-	-18.0
SCl 3	Target	5.888	5.888	-	6.869	0.455	-	15.701	4.907	-	-	13.154	-	1.998	44.160	-	-	0.981
	Meas.	6.24	5.94	-	6.39	0.318	-	14.6	4.89	-	-	12.5	-	1.08	47.9	-	-	0.838
	% Err	6.0	0.9	-	-7.0	-30.0	-	-7.0	-0.3	-	-	-5.0	-	-45.9	8.5	-	-	-14.6
SCl 4	Target	5.871	5.871	-	6.850	0.606	-	15.655	4.892	-	-	13.249	-	1.997	44.030	-	-	0.979
	Meas.	6.24	6.07	-	6.58	0.421	-	14.6	4.88	-	-	12.6	-	1.04	47.8	-	-	0.845
	% Err	6.3	3.4	-	-3.9	-30.5	-	-6.7	-0.3	-	-	-4.9	-	-47.9	8.6	-	-	-13.7
SCl 5	Target	5.802	5.802	-	6.770	1.210	-	15.473	4.835	-	-	13.629	-	1.995	43.517	-	-	0.967
	Meas.	7.2	5.97	-	6.39	0.777	-	14.1	4.83	-	-	12.6	-	0.835	47.6	-	-	0.807
	% Err	24.1	2.9	-	-5.6	-35.8	-	-8.9	-0.1	-	-	-7.6	-	-58.1	9.4	-	-	-16.6
A3=B3+S	Target	5.939	5.939	-	6.929	-	-	15.838	4.950	-	-	12.869	-	2.000	44.546	-	-	0.990
	Meas.	6.34	6.18	-	6.46	-	-	14.3	4.97	-	-	12	-	1.12	48.1	-	-	0.889
	% Err	6.8	4.1	-	-6.8	-	-	-9.7	0.4	-	-	-6.8	-	-44.0	8.0	-	-	-10.2
SV 1	Target	5.788	5.788	-	6.753	-	-	15.435	4.823	-	-	12.541	-	2	43.41	2.5	-	0.965
	Meas.	6.47	4.87	-	6.67	-	-	15.0	4.54	-	-	12.1	-	1.50	46.6	2.35	-	0.833
	% Err	11.8	-15.9	-	-1.2	-	-	-2.8	-5.9	-	-	-3.5	-	-25.0	7.3	-6.0	-	-13.7
SV 2	Target	5.636	5.636	-	6.576	-	-	15.031	4.697	-	-	12.212	-	2	42.274	5	-	0.939
	Meas.	5.84	4.76	-	5.76	-	-	13.8	4.47	-	-	11.7	-	1.68	48.0	4.42	-	0.841
	% Err	3.6	-15.5	-	-12.4	-	-	-8.2	-4.8	-	-	-4.2	-	-16.0	13.5	-11.6	-	-10.4
SV 3	Target	5.485	5.485	-	6.4	-	-	14.626	4.571	-	-	11.884	-	2	41.136	7.5	-	0.914
	Meas.	5.94	4.37	-	5.89	-	-	12.8	4.19	-	-	11.4	-	1.79	48.0	6.34	-	0.731
	% Err	8.3	-20.3	-	-8.0	-	-	-12.5	-8.3	-	-	-4.1	-	-10.5	16.7	-15.5	-	-20.0
SV 4	Target	5.333	5.333	-	6.222	-	-	14.222	4.444	-	-	11.556	-	2	40	10	-	0.889
	Meas.	5.90	4.29	-	6.25	-	-	14.0	4.46	-	-	11.2	-	2.23	44.3	9.33	-	0.819
	% Err	10.6	-19.6	-	0.5	-	-	-1.6	0.4	-	-	-3.1	-	11.5	10.8	-6.7	-	-7.9
A3B3+S	Target	5.939	5.939	-	6.929	-	-	15.838	4.95	-	-	12.869	-	2	44.546	-	-	0.99
	Meas.	6.53	4.90	-	6.79	-	-	15.2	4.70	-	-	12.2	-	1.23	47.7	-	-	0.921
	% Err.	10.0	-17.5	-	-2.0	-	-	-4.0	-5.1	-	-	-5.2	-	-38.5	7.1	-	-	-7.0

Table A-2. Comparison of Targeted and Measured Compositions (wt %) of the Study Glasses (continued)

ID	Type	Al_2O_3	B_2O_3	BaO	CaO	Cl	Cr_2O_3	Fe_2O_3	Li_2O	MgO	MnO	Na_2O	P_2O_5	SO_3	SiO_2	V_2O_5	ZnO	ZrO_2
S Fe 1	Target	6.072	6.072	-	7.084	-	-	14	5.06	-	-	13.157	-	2	45.542	-	-	1.012
	Meas.	6.92	4.97	-	6.80	-	-	13.6	4.83	-	-	12.4	-	1.28	49.1	-	-	0.929
	% Err	14.0	-18.1	-	-4.0	-	-	-2.9	-4.5	-	-	-5.8	-	-36.0	7.8	-	-	-8.2
S Fe 2	Target	6.289	6.289	-	7.337	-	-	11	5.241	-	-	13.627	-	2	47.169	-	-	1.048
	Meas.	7.17	5.12	-	6.99	-	-	10.9	5.00	-	-	13.0	-	1.29	50.8	-	-	0.960
	% Err	14.0	-18.6	-	-4.7	-	-	-0.9	-4.6	-	-	-4.6	-	-35.5	7.7	-	-	-8.4
S Fe 3	Target	6.506	6.506	-	7.59	-	-	8	5.422	-	-	14.096	-	2	48.795	-	-	1.084
	Meas.	7.43	5.36	-	7.33	-	-	8.15	5.19	-	-	13.6	-	1.30	52.3	-	-	1.01
	% Err	14.2	-17.6	-	-3.4	-	-	1.9	-4.3	-	-	-3.5	-	-35.0	7.2	-	-	-6.8
S Fe 4	Target	6.723	6.723	-	7.843	-	-	5	5.602	-	-	14.566	-	2	50.422	-	-	1.12
	Meas.	6.91	5.39	-	7.51	-	-	5.33	5.36	-	-	13.8	-	1.54	53.8	-	-	0.995
	% Err	2.8	-19.8	-	-4.2	-	-	6.6	-4.3	-	-	-5.3	-	-23.0	6.7	-	-	-11.2

Distribution:

J. W. Amoroso, 999-W
H. P. Boyd, 707-7E
J. M. Bricker, 704-S
T. B. Brown, 773-A
H. H. Burns, 773-41A
M. J. Cercy, 773-42A
A. S. Choi, 999-W
A. D. Cozzi, 999-W
C. L. Crawford, 773-42A
D. E. Dooley, 999-W
R. E. Edwards, 766-H
T. B. Edwards, 999-W
A. P. Fellinger. 773-42A
T. L. Fellinger, 766-H
S. D. Fink, 773-A
K. M. Fox, 999-W
E. J. Freed, 704-S
J. C. Griffin, 773-A
E. K. Hansen, 999-W
C. C. Herman, 773-A
E. N. Hoffman, 999-W
E. W. Holtzscheiter, 766-H
J. E. Hyatt, 773-A
J. F. Iaukea, 704-27S
V. Jain, 766-H
C. M. Jantzen, 773-A
F. C. Johnson, 999-W
D. S. Kim, PNNL
C. J. Martino, 999-W
D. J. McCabe, 773-42A
D. L. McClane, 999-W
D. H. McGuire, 999-W
R. T. McNew, 766-H
D. H. Miller, 999-W
F. M. Pennebaker, 773-42A
E. M. Pierce, ORNL
M. R. Poirier, 773-42A
M. A. Rios-Armstrong, 766-H
H. B. Shah, 766-H
D. C. Sherburne, 704-126S
M. E. Stone, 999-W
C. L. Trivelpiece, 999-W
J. D. Vienna, PNNL
J. R Vitali, 704-30S
B. J. Wiedenman, 773-42A
W. R. Wilmarth, 773-A
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